

Aleksandr A Shubin

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/1398950/publications.pdf>

Version: 2024-02-01

95
papers

1,925
citations

236833

25
h-index

289141

40
g-index

97
all docs

97
docs citations

97
times ranked

1739
citing authors

#	ARTICLE	IF	CITATIONS
1	51V Solid state NMR studies of vanadia based catalysts. Progress in Nuclear Magnetic Resonance Spectroscopy, 1992, 24, 457-525.	3.9	180
2	Water Concentration Profiles in Membranes Measured by ESEEM of Spin-Labeled Lipids. Journal of Physical Chemistry B, 2005, 109, 12003-12013.	1.2	116
3	Practical aspects of 51V and 93Nb solid-state NMR spectroscopy and applications to oxide materials. Progress in Nuclear Magnetic Resonance Spectroscopy, 2008, 53, 128-191.	3.9	85
4	DFT study of oxygen-bridged Zn ²⁺ ion pairs in Zn/ZSM-5 zeolites. Catalysis Letters, 2000, 70, 175-181.	1.4	83
5	The metallocene/methylaluminoxane catalysts formation: EPR spin probe study of Lewis acidic sites of methylaluminoxane. Journal of Molecular Catalysis A, 1999, 139, 131-137.	4.8	63
6	Characterization of V ₂ O ₅ ~TiO ₂ Catalysts Prepared by Milling by ESR and Solid State 1H and 51V NMR. Journal of Physical Chemistry B, 1999, 103, 7599-7606.	1.2	51
7	Comparative Quantum Chemical Study of Stabilization Energies of Zn ²⁺ Ions in Different Zeolite Structures. Journal of Physical Chemistry B, 2001, 105, 4928-4935.	1.2	51
8	Antimony Oxide-Modified Vanadia-Based Catalysts Physical Characterization and Catalytic Properties. Journal of Physical Chemistry B, 2001, 105, 10772-10783.	1.2	49
9	Theoretical and experimental insights into applicability of solid-state 93Nb NMR in catalysis. Physical Chemistry Chemical Physics, 2013, 15, 5115.	1.3	48
10	DFT Cluster Modeling of Molecular and Dissociative Hydrogen Adsorption on Zn ²⁺ Ions with Distant Placing of Aluminum in the Framework of High-Silica Zeolites. Catalysis Letters, 2003, 90, 137-142.	1.4	45
11	Modulation effects in the electron spin echo resulting from hyperfine interaction with a nucleus of an arbitrary spin. Journal of Magnetic Resonance, 1981, 42, 474-487.	0.5	44
12	Composition of the active component of supported vanadium-magnesium catalysts according to 51 NMR data. Journal of Molecular Catalysis, 1989, 50, 55-65.	1.2	44
13	EPR Monitoring of Vanadium(IV) Species Formed upon Activation of Vanadium(V) Polyphenolate Precatalysts with AlR ₂ Cl and AlR ₂ Cl/Ethyltrichloroacetate (R = Me, Et). Organometallics, 2009, 28, 6714-6720.	1.1	43
14	Characterisation of strongly bonded V(V) species in VO/TiO ₂ catalyst by static and MAS solid-state NMR spectroscopy. Chemical Physics Letters, 1999, 302, 341-346.	1.2	41
15	Solid-state NMR for characterization of vanadium-containing systems. Catalysis Today, 2003, 78, 91-104.	2.2	41
16	Spectroscopic identification of adsorption properties of Zn ²⁺ ions at cationic positions of high-silica zeolites with distant placing of aluminium ions. Theoretical Chemistry Accounts, 2005, 114, 90-96.	0.5	39
17	Radical Intermediates in the Photoinduced Formation of Benzene Cation-Radicals over H-ZSM-5 Zeolites. The Journal of Physical Chemistry, 1994, 98, 7551-7554.	2.9	36
18	Effect of Milling of V ₂ O ₅ on the Local Environment of Vanadium as Studied by Solid-State 51V NMR and Complementary Methods. Journal of Physical Chemistry B, 1999, 103, 3138-3144.	1.2	36

#	ARTICLE	IF	CITATIONS
19	Raman identification of lonsdaleite in Popigai impactites. <i>Journal of Raman Spectroscopy</i> , 2014, 45, 305-313.	1.2	36
20	ESEEM Measurements of Local Water Concentration in D2O-Containing Spin-Labeled Systems. <i>Applied Magnetic Resonance</i> , 2008, 35, 73-94.	0.6	35
21	Molecular Dynamics of n-Octane Inside Zeolite ZSM-5 As Studied by Deuterium Solid-State NMR and Quasi-Elastic Neutron Scattering. <i>Journal of Physical Chemistry B</i> , 1998, 102, 10860-10870.	1.2	32
22	Possible molecular structure of promoted Lewis acidity sites in ZnZSM-5. <i>International Journal of Quantum Chemistry</i> , 2004, 100, 489-494.	1.0	32
23	⁵¹ V and ³¹ P NMR studies of VOx/TiO2 catalysts modified by phosphorous. <i>Journal of Molecular Catalysis A</i> , 2000, 162, 381-390.	4.8	30
24	An EPR Study of the V(IV) Species Formed Upon Activation of a Vanadyl Phenoxyimine Polymerization Catalyst with AlR ₃ and AlR ₂ Cl (R = Me, Et). <i>Macromolecular Chemistry and Physics</i> , 2009, 210, 542-548.	1.1	28
25	Characterization by solid state ⁵¹ V NMR spectroscopy. <i>Catalysis Today</i> , 2000, 56, 379-387.	2.2	26
26	Relation between catalyst structure and selectivity of the oxidative coupling of 2,6-dimethylphenol in the presence of copper complexes: studies using EPR and NMR. <i>Journal of Molecular Catalysis</i> , 1990, 57, 325-351.	1.2	25
27	Dynamics of Isobutane inside Zeolite ZSM-5. A Study with Deuterium Solid-State NMR. <i>Journal of Physical Chemistry B</i> , 2002, 106, 10114-10120.	1.2	25
28	A comparative, two-dimensional ¹⁴ N ESEEM characterization of reduced [2Fe-2S] clusters in hyperthermophilic archaeal high- and low-potential Rieske-type proteins. <i>Journal of Biological Inorganic Chemistry</i> , 2004, 9, 753-767.	1.1	25
29	High-resolution solid-state magic angle spinning nuclear magnetic resonance investigations of surface hydroxy groups on modified silica gel. <i>Journal of the Chemical Society Faraday Transactions I</i> , 1986, 82, 1879.	1.0	22
30	A computational study of the adsorption of the isomers of butanol on silicalite and H-ZSM-5. <i>Proceedings of the Royal Society A</i> , 1994, 446, 411-427.	1.0	22
31	Study of nature of the factors determining activity, stability and selectivity of zeolite catalyst. <i>Zeolites</i> , 1984, 4, 114-119.	0.9	21
32	Dynamics of n-Hexane Inside Silicalite, As Studied by ² H NMR. <i>Journal of Physical Chemistry B</i> , 2003, 107, 7095-7101.	1.2	21
33	Molecular Dynamics of iso-Butyl Alcohol Inside Zeolite H-ZSM-5 as Studied by Deuterium Solid-State NMR Spectroscopy. <i>Journal of Physical Chemistry B</i> , 2000, 104, 7677-7685.	1.2	20
34	Exploring by Pulsed EPR the Electronic Structure of Ubisemiquinone Bound at the QH Site of Cytochrome bo3 from Escherichia coli with in Vivo ¹³ C-Labeled Methyl and Methoxy Substituents. <i>Journal of Biological Chemistry</i> , 2011, 286, 10105-10114.	1.6	20
35	Multinuclear NMR studies of V2O5-Cs2S2O7 melts. <i>Journal of Molecular Catalysis A</i> , 1995, 99, 123-130.	4.8	19
36	Proton Environment of Reduced Rieske Iron-Sulfur Cluster Probed by Two-Dimensional ESEEM Spectroscopy. <i>Journal of Physical Chemistry A</i> , 2009, 113, 653-667.	1.1	19

#	ARTICLE	IF	CITATIONS
37	The influence of nuclear quadrupole interactions upon electron spin-echo modulation induced by weak hyperfine interactions. <i>Journal of Magnetic Resonance</i> , 1983, 52, 1-12.	0.5	17
38	Cluster Model DFT Study of CO Adsorption to Gallium Ions in Ga/HZSM-5. <i>Journal of Physical Chemistry C</i> , 2008, 112, 3321-3326.	1.5	17
39	The impact of framework flexibility and defects on the water adsorption in CAU-10-H. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 21329-21337.	1.3	17
40	Electron Paramagnetic Resonance Study of the Interaction of Surface Titanium Species with AlR ₃ Cocatalyst in Supported Ziegler-Natta Catalysts with a Low Titanium Content. <i>Journal of Physical Chemistry C</i> , 2016, 120, 1121-1129.	1.5	16
41	Observation of two paramagnetic species in electron transfer reactions within cesium modified X and Y zeolites. <i>Chemical Physics Letters</i> , 2000, 316, 404-410.	1.2	15
42	Hydrogen abstraction from methane on cristobalite supported W and Mn oxo complexes: A DFT study. <i>Molecular Catalysis</i> , 2018, 445, 307-315.	1.0	15
43	High-Temperature NMR Studies of the Glass-Crystal Transition in the Cs ₂ S ₂ O ₇ -V ₂ O ₅ System. <i>Journal of Physical Chemistry B</i> , 1997, 101, 9188-9194.	1.2	14
44	Formation, structure, and reactivity of palladium superoxo complexes. <i>Inorganic Chemistry</i> , 1987, 26, 3871-3878.	1.9	13
45	EPR and ¹ H NMR spectroscopic characterization of the ferric species formed in the iron picolinate/(pyridine/acetic acid)/HOOH catalytic system for the direct ketonization of methylenic carbons. <i>Journal of Molecular Catalysis A</i> , 1996, 112, 253-258.	4.8	13
46	Self-Aggregation and Orientation of the Ion Channel-Forming Zervamicin IIA in the Membranes of ePC Vesicles Studied by cw EPR and ESEEM Spectroscopy. <i>Applied Magnetic Resonance</i> , 2010, 38, 75-84.	0.6	13
47	Surface Hydroxyl OH Defects of γ-Al ₂ O ₃ and δ-Al ₂ O ₃ by Solid State NMR, XRD, and DFT Calculations. <i>Zeitschrift Fur Physikalische Chemie</i> , 2017, 231, 809-825.	1.4	13
48	Electron spin-echo modulation effects in disordered systems: Structure of traps for H and D atoms in frozen water solutions based on ¹ H and ² D nuclear modulation data. <i>Journal of Chemical Physics</i> , 1983, 79, 5785-5795.	1.2	12
49	Distinct activity of the oxyl Fe(II)O group in the methane dissociation by activated iron hydroxide: DFT predictions. <i>Chemical Physics Letters</i> , 2015, 640, 94-100.	1.2	12
50	Calculation of anisotropically broadened EPR spectra. Shape of the EPR spectrum of a nitroxide radical in the two-millimeter range. <i>Journal of Structural Chemistry</i> , 1989, 30, 414-417.	0.3	10
51	The state of Cu ²⁺ ions in concentrated aqueous ammonia solutions of copper nitrate. <i>Russian Journal of Inorganic Chemistry</i> , 2012, 57, 1285-1290.	0.3	10
52	Effect of Impregnation on the Structure of Niobium Oxide/Alumina Catalysts Studied by Multinuclear Solid-State NMR, FTIR, and Quantum Chemical Calculations. <i>Journal of Physical Chemistry C</i> , 2015, 119, 10400-10411.	1.5	10
53	The routes of association of (hydro)oxo centers on iron hydroxide at the water oxidation process: DFT predictions. <i>Chemical Physics Letters</i> , 2015, 619, 126-132.	1.2	10
54	Hidden radical reactivity of the [FeO] ₂ ⁺ group in the H-abstraction from methane: DFT and CASPT2 supported mechanism by the example of model iron (hydro)oxide species. <i>Chemical Physics Letters</i> , 2017, 679, 193-199.	1.2	10

#	ARTICLE	IF	CITATIONS
55	High-temperature multinuclear magnetic resonance studies of vanadia catalysts for SO ₂ oxidation. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 1999, 158, 255-271.	2.3	9
56	Crystal structure of copper perchlorophthalocyanine analysed by 3D electron diffraction. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2021, 77, 662-675.	0.5	9
57	Solid-state 51V NMR and its potentiality in investigation of vanadia systems with paramagnetic centres. <i>Catalysis Today</i> , 2009, 142, 220-226.	2.2	7
58	Photochemistry of Dithiocarbamate Cu(S ₂ CNEt ₂) ₂ Complex in CHCl ₃ . Transient Species and TD-DFT Calculations. <i>Journal of Physical Chemistry A</i> , 2016, 120, 7873-7880.	1.1	7
59	Pyrolysis of the Cellulose Fraction of Biomass in the Presence of Solid Acid Catalysts: An Operando Spectroscopy and Theoretical Investigation. <i>ChemSusChem</i> , 2018, 11, 4044-4059.	3.6	7
60	Numerical analysis of the influence of nuclear quadrupole interaction on modulation effects in electron spin echo from deuterium nuclei in disordered systems. <i>Journal of Magnetic Resonance</i> , 1985, 64, 185-193.	0.5	6
61	Variations of g-tensor principal values in reduced [2Fe ²⁺ 2S] cluster of iron-sulfur proteins. <i>Applied Magnetic Resonance</i> , 2006, 30, 399-416.	0.6	6
62	Specific features of association of Cu ²⁺ ions in concentrated aqueous ammonia solutions of copper nitrate as probed by ESR. <i>Doklady Physical Chemistry</i> , 2011, 440, 194-197.	0.2	6
63	Oxidation of Water to Molecular Oxygen by One-Electron Oxidants on Transition Metal Hydroxides. <i>Kinetics and Catalysis</i> , 2018, 59, 23-47.	0.3	6
64	Oxygen transport in Pr nickelates: Elucidation of atomic-scale features. <i>Solid State Ionics</i> , 2020, 344, 115155.	1.3	6
65	O ₂ ⁻ anion radical in the coordination sphere of palladium in solution. <i>Reaction Kinetics and Catalysis Letters</i> , 1986, 31, 209-214.	0.6	5
66	The structure of zirconium-silicate fibreglasses and Pt-containing fiberglass catalysts as revealed by solid-state NMR spectroscopy. <i>Journal of Structural Chemistry</i> , 2013, 54, 152-167.	0.3	5
67	Entropy driven preference for alkene adsorption at the pore mouth as the origin of pore-mouth catalysis for alkane hydroisomerization in 1D zeolites. <i>Catalysis Science and Technology</i> , 2021, 11, 563-574.	2.1	5
68	Ln(III) complexes with a chiral 1 <i>H</i> -pyrazolo[3,4- <i>b</i>]pyridine derivative fused with a (1 <i>R</i>)-1 <i>π</i> -pinene moiety: synthesis, crystal structure, and photophysical studies in solution and in the solid state. <i>New Journal of Chemistry</i> , 2021, 45, 2276-2284.	1.4	5
69	A novel adsorption-based method for revealing the Si distribution in SAPO molecular sieves: The case of SAPO-11. <i>Microporous and Mesoporous Materials</i> , 2021, 328, 111503.	2.2	5
70	A study of polyhedral octa (organosilasesquioxanes) by high-resolution NMR at the ¹³ C and ²⁹ Si nuclei in the solid state. <i>Journal of Structural Chemistry</i> , 1982, 23, 345-348.	0.3	4
71	Condensation of ammonium niobium oxalate studied by NMR crystallography and X-ray powder diffraction. <i>Catalysis Today</i> , 2020, 354, 26-35.	2.2	4
72	Adsorption properties of oxidized gallium-modified zeolite ZSM-5 from diffuse-reflectance IR-spectroscopic and quantum-chemical data: II. Interaction with carbon monoxide and water. <i>Kinetics and Catalysis</i> , 2008, 49, 149-155.	0.3	3

#	ARTICLE	IF	CITATIONS
73	First principles calculation of the stacking fault in (111) low-temperature metastable alumina. Journal of Structural Chemistry, 2016, 57, 294-300.	0.3	3
74	Influence of Polarity and Ionic Strength on Intramolecular Spin Exchange in a Short Nitroxide Biradical, Containing Sulphur Atom in the Bridge. Applied Magnetic Resonance, 2018, 49, 1059-1073.	0.6	3
75	Photochemistry of dithiophosphinate Ni(S ₂ P(i-Bu) ₂) ₂ complex in CCl ₄ . Transient species and TD-DFT calculations. Journal of Photochemistry and Photobiology A: Chemistry, 2019, 381, 111857.	2.0	3
76	Change in sign of exchange integral in conformational transition in molecule of stable nitroxyl diradical. Bulletin of the Academy of Sciences of the USSR Division of Chemical Science, 1981, 30, 1660-1663.	0.0	2
77	²³ Na NMR study of the mechanism for the dehydration of zeolite NaA. Bulletin of the Academy of Sciences of the USSR Division of Chemical Science, 1988, 37, 1020-1022.	0.0	2
78	Orbital ordering of Cu ²⁺ ions in concentrated aqueous ammonia solutions of copper chloride, sulfate, and acetate as probed by ESR. Doklady Physical Chemistry, 2013, 450, 103-106.	0.2	2
79	Random Distribution of EFG Parameters in ²⁷ Al MAS NMR Spectra of AlO _x /SiO ₂ Catalysts and Related Systems. Applied Magnetic Resonance, 2016, 47, 1193-1205.	0.6	2
80	Solid-State NMR of Oxide-Based Materials. , 2018, , 1125-1160.		2
81	Reactivity Theory of Zinc Cation Species in Zeolites. , 2001, , 187-204.		2
82	Factors affecting the stability and selectivity of zeolites in the conversion of methanol to hydrocarbons. Communication 2. Effect of dealuminization. Bulletin of the Academy of Sciences of the USSR Division of Chemical Science, 1986, 35, 909-913.	0.0	1
83	ESR spectra of oxygen radical-ions in kaolinite. Journal of Structural Chemistry, 1992, 33, 151-153.	0.3	1
84	ESR study of ordered Ti(III) clusters in frozen solutions. Reaction Kinetics and Catalysis Letters, 1994, 52, 261-267.	0.6	1
85	EPR-spectroscopic detection and characterization of a CuII complex with a peroxy-carboximidic acid. Mendeleev Communications, 2001, 11, 206-207.	0.6	1
86	Determination of Hyperfine Tensor Components from Nuclear Frequencies at Canonical Orientations of the g-Tensor. Journal of Magnetic Resonance, 2002, 155, 100-105.	1.2	1
87	On the nature of radicals formed in methanol catalytic oxidation. Kinetics and Catalysis, 2009, 50, 583-586.	0.3	1
88	DFT predictions for hydrogen atom transfer at the [FeO] ₂ ⁺ group: A distinct activity of the oxyl state FeIII-O [•] . AIP Conference Proceedings, 2016, , .	0.3	1
89	Identification of beryllium fluoride complexes in mechanically distorted gels using quadrupolar split ⁹ Be NMR spectra resolved with solution-state selective cross-polarization. Physical Chemistry Chemical Physics, 2021, 23, 16932-16941.	1.3	1
90	Investigation of vanadia [•] -alumina catalysts with solid-state NMR spectroscopy and DFT. Physical Chemistry Chemical Physics, 2021, 23, 19352-19363.	1.3	1

#	ARTICLE	IF	CITATIONS
91	Spatial organization of random coils of linear poly(ethylenimine) containing copper(II) ions in solution. <i>Journal of Structural Chemistry</i> , 1989, 30, 260-267.	0.3	0
92	Solid-State NMR of Oxide-Based Materials. , 2016, , 1-37.		0
93	Photophysical processes for phenanthroline-menthol ligand and its Eu(III) and Tb(III) complexes in solution. <i>Journal of Luminescence</i> , 2019, 214, 116548.	1.5	0
94	Integral Intensity of the EPR Signal of NO Molecules Adsorbed on Lewis Acid Sites of Oxide Systems as a Function of Surface Coverage. <i>Applied Magnetic Resonance</i> , 2020, 51, 993-1003.	0.6	0
95	The Fe IV μ_2 O μ_2 oxyl unit as a key intermediate in water oxidation on the Fe III μ_2 hydroxide: DFT predictions. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26610.	1.0	0